

The Ordering Ambiguity

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Abstract: The kinetic energy operator of a quantum particle with position dependent mass and the associated ordering ambiguity is revisited. We introduce a new form of this operator which is a continues or discreet superposition of the acceptable values for the ordering parameters.

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I. INTRODUCTION

Position-dependent-mass (PDM) particles have received interests over the last few decades [1]. From the very beginning, parallel to the applicability of the PDM-settings in different areas of physics such as the many-body problem [2], semiconductors [3], quantum dots [4], quantum liquids [5], He-Clusters [6], etc. a mathematical difficulty has grown which is known as *the ordering ambiguity*. Von-Roos has, firstly, reported the problem by proposing the revolutionary form of the PDM kinetic energy operator which reads as [7]

$$\hat{T} = \frac{1}{4} (m^\alpha \hat{p} m^\beta \hat{p} m^\gamma + m^\gamma \hat{p} m^\beta \hat{p} m^\alpha). \quad (1)$$

Here m is the position dependent mass of the physical particle and α , β and γ are some real parameters which satisfy the constraint $\alpha + \beta + \gamma = -1$. In the constant mass setting, (1) reduces to the standard kinetic energy operator which is given by

$$\hat{T} = \frac{\hat{p}^2}{2m}. \quad (2)$$

We note that in Eq. (1), although $\alpha + \beta + \gamma = -1$ but the exact values of α , β and γ are not known and without any harm to the mathematics of the problem, this von-Roos parameters may accept any real number. The nature of the problem turns to the fact that the momentum operator \hat{p} does not commute with the position operator \hat{x} in quantum theory.

In the literature, there exist several suggestions for the von-Roos ordering parameters, for instance, the Gora's and Williams' ($\beta = \gamma = 0$, $\alpha = -1$) [8], Ben Daniel's and Duke's ($\alpha = \gamma = 0$, $\beta = -1$) [9], Zhu's and Kroemer's ($\alpha = \gamma = -1/2$, $\beta = 0$) [10], Li's and Kuhn's ($\alpha = 0$, $\beta = \gamma = -1/2$) [11], and the very recent Mustafa's and Mazharimousavi's ($\alpha = \gamma = -1/4$, $\beta = -1/2$) [12]. It has been observed that the physical admissibility of a given ambiguity parameters set very well depends not only on the continuity conditions at the abrupt heterojunction boundaries but also on the position-dependent-mass form. The general consensus is that there is no unique and universal choice for these ambiguity parameters.

II. CONTINUES ORDERING PARAMETERS

The idea which we shall expand in the sequel, is to construct a quantum kinetic operator which is a superposition of all possible values for the von-Roos parameters α , β and γ . In doing so, we also introduce a weight function which gives the distribution of the different ordering parameters. The idea can be developed in two different directions: i) a continues distribution and ii) a discrete distribution. Here in this section we study the continues distribution and in the next section, the discrete distribution will be given.

Following to our proposal we introduce the kinetic energy operator \hat{T} for a position dependent mass particle as

$$\hat{T} = \frac{1}{4A} \iint_{\mathcal{R}} dA \rho(\alpha, \beta) (m^\alpha \hat{p} m^\beta \hat{p} m^\gamma + m^\gamma \hat{p} m^\beta \hat{p} m^\alpha) \quad (3)$$

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in which $\rho(\alpha, \beta) : \mathbb{R}^2 \rightarrow \mathbb{R}$ is the weight function, dA is the surface element on $\alpha - \beta$ plane and

$$A = \iint_{\mathcal{R}} dA \rho(\alpha, \beta) \quad (4)$$

can be called a normalization constant (see Fig. 1 and 2).

We note that the third parameter γ , is not free and therefore, the integral is taken only over two of the parameters (i.e., α and β). Furthermore, one may impose additional conditions on these parameters to specify the domain of the ordering parameters, for instance, $\alpha, \beta, \gamma \in [-1, 0]$. Latter constraint looks to be reasonable because, the well-known ordering-parameter sets available in the literature, belong to this domain. In spite of this fact, we keep the parameters free, to get any values in \mathbb{R} , but under a rather flexible constraint.

Let's consider the domain of α, β and γ the same and fully symmetric which we called them $\mathcal{R}_1, \mathcal{R}_2 \dots$ (Fig. 2). In this figure, \mathcal{R}_i is located on the plane $\alpha + \beta + \gamma = -1$ in the space of α, β and γ . In addition to \mathcal{R}_i we also introduce \mathcal{R} to be the projection of \mathcal{R}_i on the plane of $\alpha - \beta$. Finally, we consider \mathcal{R}_i , an equilateral triangle which leads to

$$\mathcal{R} = \begin{cases} -(1+b) \leq \alpha \leq \frac{b}{2} \\ -(1+\frac{b}{2}+\alpha) \leq \beta \leq \frac{b}{2} \end{cases} \quad (5)$$

in which $-\frac{2}{3} \leq b \in \mathbb{R}$ and it shows the size of the region \mathcal{R}_i .

By considering the natural unit, i.e., $\hbar = 1$, one finds

$$\begin{aligned} m^\alpha \hat{p} m^\beta \hat{p} m^\gamma + m^\gamma \hat{p} m^\beta \hat{p} m^\alpha = \\ -2 \left((1+\alpha+\beta+\alpha\beta+\alpha^2) \frac{m'^2}{m^3} - \frac{1}{2} (1+\beta) \frac{m''}{m^2} - \frac{m'}{m^2} \partial_x + \frac{1}{m} \partial_x^2 \right), \end{aligned} \quad (6)$$

which yields

$$\hat{T} = -\frac{1}{2A} \iint_{\mathcal{R}} dA \rho(\alpha, \beta) \left((1+\alpha+\beta+\alpha\beta+\alpha^2) \frac{m'^2}{m^3} - \frac{1}{2} (1+\beta) \frac{m''}{m^2} - \frac{m'}{m^2} \partial_x + \frac{1}{m} \partial_x^2 \right). \quad (7)$$

A. A UNIFORM DISTRIBUTION

As an example, we study the case of $\rho(\alpha, \beta) = 1$ which is a uniform and symmetric distribution. By setting $\rho(\alpha, \beta) = 1$ in Eq. (7) it leads to

$$\hat{T} = \frac{-1}{6} \left(\frac{1}{16} (3b^2 + 4b + 28) \frac{m'^2}{m^3} - \frac{m''}{m^2} \right) + \frac{1}{2} \left(\frac{m'}{m^2} \partial_x - \frac{1}{m} \partial_x^2 \right). \quad (8)$$

It is remarkable to observe that for $\forall b \in [-\frac{2}{3}, \infty)$ non of the first two terms are zero. We note that among the possible values for b , $b = -\frac{2}{3}$ corresponds to

$$\alpha = \beta = \gamma = -\frac{1}{3}. \quad (9)$$

This set of parameters consequently implies

$$\hat{T} = \frac{-1}{2} \left(\frac{5}{9} \frac{m'^2}{m^3} - \frac{1}{3} \frac{m''}{m^2} \right) + \frac{1}{2} \left(\frac{m'}{m^2} \partial_x - \frac{1}{m} \partial_x^2 \right). \quad (10)$$

Another interesting case is when $b = 0$, which makes α, β and γ lie in the interval $[-1, 0]$. The kinetic energy after setting $b = 0$ reads

$$\hat{T} = \frac{-1}{6} \left(\frac{7}{4} \frac{m'^2}{m^3} - \frac{m''}{m^2} \right) + \frac{1}{2} \left(\frac{m'}{m^2} \partial_x - \frac{1}{m} \partial_x^2 \right). \quad (11)$$

B. A NON-UNIFORM DISTRIBUTION

Next we give an example with the non-uniform distribution function $\rho(\alpha, \beta)$ which is given by

$$\rho(\alpha, \beta) = \frac{1}{(\alpha^2 + 1)} + \frac{1}{(\beta^2 + 1)}. \quad (12)$$

This is a symmetric distribution with respect to α and β . Consequently the form of kinetic energy becomes

$$\hat{T} = -\frac{1}{2} \left(\eta_1 \frac{m'^2}{m^3} + \eta_2 \frac{m''}{m^2} - \frac{m'}{m^2} \partial_x + \frac{1}{m} \partial_x^2 \right), \quad (13)$$

where

$$\eta_1 = \frac{-(3b^2 + 12b + 20) \ln \left(\frac{4(2+2b+b^2)}{4+b^2} \right) + 2(b^3 + 3b^2 + 12b + 4) (\tan^{-1} \frac{b}{2} + \tan^{-1}(1+b)) + 15b^2 + 40b + 20}{48(1+b) (\tan^{-1} \frac{b}{2} + \tan^{-1}(1+b)) - 24 \ln \left(\frac{4(2+2b+b^2)}{4+b^2} \right)}, \quad (14)$$

and

$$\eta_2 = \frac{(b+4) \ln \left(\frac{4(2+2b+b^2)}{4+b^2} \right) + 2(3b+2) (\tan^{-1} \frac{b}{2} + \tan^{-1}(1+b)) - (3b+2)}{16(1+b) (\tan^{-1} \frac{b}{2} + \tan^{-1}(1+b)) - 8 \ln \left(\frac{4(2+2b+b^2)}{4+b^2} \right)} \quad (15)$$

One can check that

$$\lim_{b \rightarrow (-\frac{2}{3})^+} \eta_1 = \frac{5}{9}, \quad (16)$$

and

$$\lim_{b \rightarrow (-\frac{2}{3})^+} \eta_2 = -\frac{1}{3} \quad (17)$$

which are exactly as we expected for $\alpha = \beta = \gamma = -\frac{1}{3}$. Also for the case of $b = 0$ one gets

$$\eta_1 = \frac{\pi + 10(1 - \ln 2)}{6(\pi - 2 \ln 2)} = 0.58966, \quad \eta_2 = -\frac{\pi + 2 - 4 \ln 2}{4(\pi - 2 \ln 2)} = -0.33746. \quad (18)$$

III. DISCRETE ORDERING PARAMETERS

As we mentioned before, there are some well-known ordering-parameters sets [8–12] which have been used widely in the literatures. These different sets which have been introduced for various physical problems, could be an indication of having a discrete ordering parameters. In this line let's introduce the kinetic energy operator with discrete distribution as

$$\hat{T} = \frac{\sum_{\alpha, \beta} C_{\alpha, \beta} (m^\alpha \hat{p} m^\beta \hat{p} m^\gamma + m^\gamma \hat{p} m^\beta \hat{p} m^\alpha)}{4 \sum_{\alpha, \beta} C_{\alpha, \beta}}, \quad (19)$$

in which $C_{\alpha, \beta}$ is a real number which can be called distribution number. We again recall that $\gamma = -1 - \alpha - \beta$ and in the summation γ is not a free index. Very similar to the case of continuous distribution one may rewrite

$$\hat{T} = -\frac{1}{2} \frac{\sum_{\alpha, \beta} C_{\alpha, \beta} \left[(1 + \alpha + \beta + \alpha\beta + \alpha^2) \frac{m'^2}{m^3} - \frac{1}{2} (1 + \beta) \frac{m''}{m^2} - \frac{m'}{m^2} \partial_x + \frac{1}{m} \partial_x^2 \right]}{\sum_{\alpha, \beta} C_{\alpha, \beta}}. \quad (20)$$

To see how this may work, we consider an equal possibility for all known ordering given before, i.e., i) Gora and Williams ($\beta = \gamma = 0, \alpha = -1$), ii) Ben Danial and Duke ($\alpha = \gamma = 0, \beta = -1$), iii) Zhu and Kroemer ($\alpha = \gamma = -1/2, \beta = 0$), iv) Li and Kuhn ($\alpha = 0, \beta = \gamma = -1/2$) and v) Mustafa and Mazharimousavi ($\alpha = -1/4, \beta = -1/2 = -1/4$). Considering these values into (20) and setting $C_{\alpha,\beta} = 1$, we find

$$\sum_{\alpha,\beta} C_{\alpha,\beta} = 5 \quad (21)$$

and consequently

$$\hat{T} = -\frac{1}{10} \left(\frac{43}{16} \frac{m'^2}{m^3} - \frac{3}{2} \frac{m''}{m^2} \right) + \frac{1}{2} \left(\frac{m'}{m^2} \partial_x - \frac{1}{m} \partial_x^2 \right). \quad (22)$$

IV. CONCLUSION

In this Letter, we have considered the long standing ordering ambiguity problem associated to the von-Roos kinetic energy operator for PDM particles. A superposition of the possible values of the von-Roos parameters has been used to construct a general kinetic energy operator. We have also introduced the distribution function which can be continues or discreet. We believe that this kinetic energy operator can assist the theoretical physicists to adjust their results along the line of the relevant experiments. In the other words there would be more free parameters in the theoretical calculations.

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Figure Captions:

Fig. 1: The plane of $\alpha + \beta + \gamma = -1$ in the space of $\alpha\beta\gamma$. The surface element on this plane is given too.

Fig. 2: The possible symmetric regions of α , β and γ on the plane of $\alpha + \beta + \gamma = -1$. The projection of these regions on $\alpha\beta$ -plane is give by (5).

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